An Implicit Thermomechanical Composite Model of PBX 9501

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The high explosive PBX 9501 is an aggregate composite composed of approximately 93 volume % HMX crystals and 7 volume % plasticized Estane®. The HMX phase is a mixed combination of one part fine size fraction and three parts coarse size fraction. The particle size distribution peak for the fine fraction is at approximately 5 microns whereas the coarse fraction peak is at approximately 200 microns. At room temperature the HMX crystals are in the monoclinic phase and are believed to behave largely as a brittle solid. In contrast the plasticized Estane® is a highly compliant rubbery polymer. Some small amount of dispersed void space (~ 1%) is also believed to exist in PBX 9501. Our efforts are meant to represent this material in a physically realistic but computationally practical way.

We are using a coupled thermomechanical generalized method of cells [1] composite model to represent PBX 9501. This model allows for the discrete representation of binder and HMX phases through the use of a representative volume element consisting of 8 cells. Each of the cells is assigned a material, and in the case of PBX 9501, a viscoelastic filled binder constitutive model [2] and an elastic-brittle HMX constitutive model [3, 4]. Through the use of an appropriate energy equation, thermal energy production, storage, and conduction are also accounted for. The fit of this model to the simple compression data of Thompson is given in Fig. 1. The simulation results are qualitatively consistent with the experiments; however, work is underway to more adequately represent the deformation behavior of this very complex material.

This composite model together with the two constitutive models has been implemented semi-implicitly into the commercially available finite element code ABAQUS. The implementation uses an analytic mechanical Jacobian for each constitutive model along with a rate of convergence algorithm to allow for variable time stepping. The stress and Jacobian tensors at each material point for the composite are taken to be the volume average of the each quantity in each composite cell.

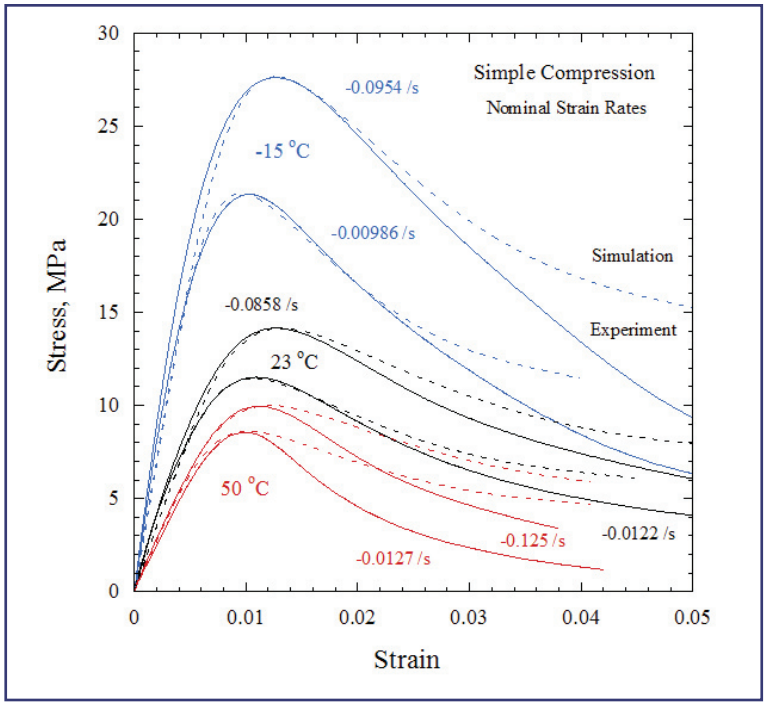

***Figure 1—** Comparison of simulation results to those of experiments used to evaluate material parameters. The red curves represent results for an initial temperature of 50˚C, the black curves for 23˚C, and the blue curves for –15˚C. The nominal strain rate for each pair of curves is also listed.*

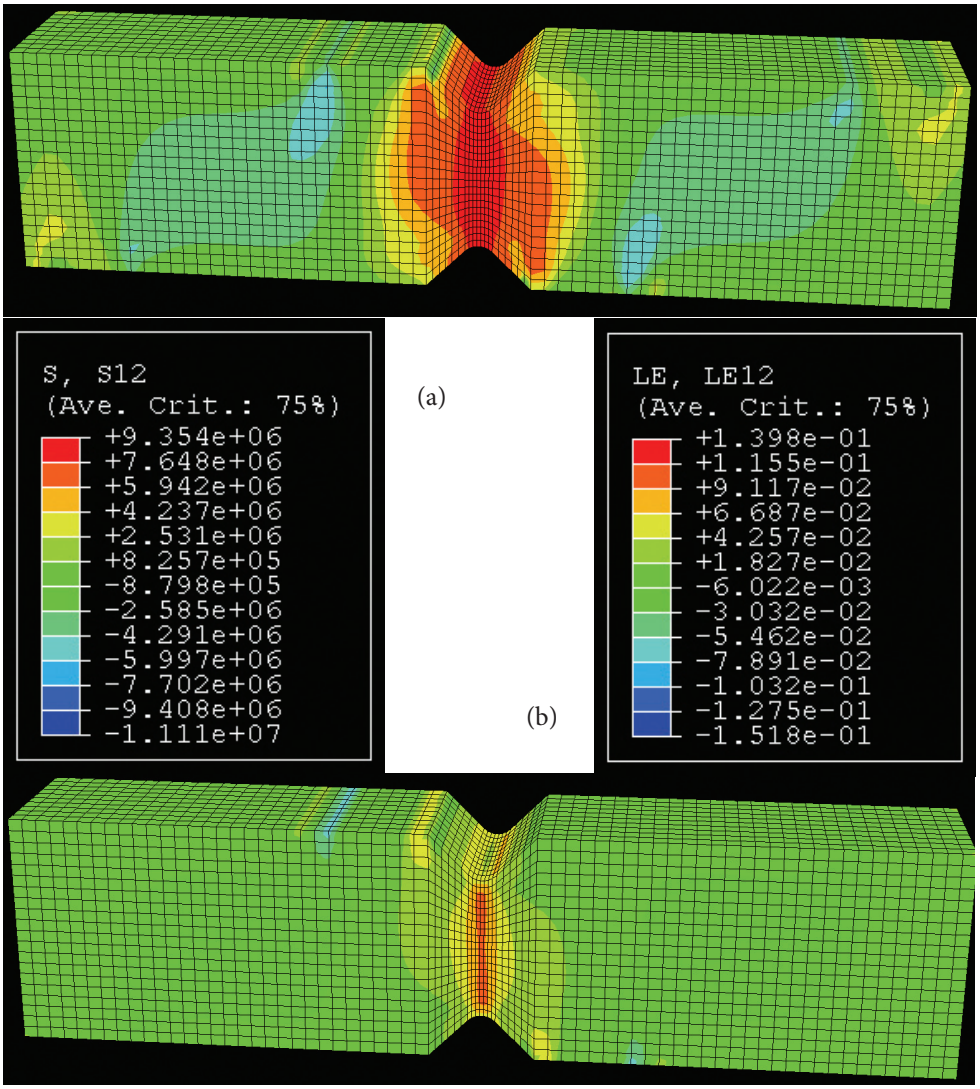

Figure 2— Three-dimensional simulation results showing (a) shear stress and (b) shear strain in a deformed Iosipescu sample of PBX 9501.

Results of a three-dimensional simulation of an Iosipescu shear sample used for PBX 9501 can be found in Fig. 2. Quantitative comparison between these simulation results and the experimental shear results of Liu [5] are currently underway.

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[2] E.M. Mas, et al., "Viscoelastic Model for PBX Binders," Los Alamos National Laboratory report LA-UR-01-3492 (June 2001).
[3] F.L. Addessio, J.N. Johnson, *J. Appl. Phys.* **67**, 3275 (1990).
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[5] C. Liu, personal communication.

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